On the connection between classical and quantum descriptions

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Abstract

The paper develops the idea that the dynamics of both classical and quantum processes is time reversible. It is shown how this classical analogy allows one to define the measure for the path integral in quantum mechanics.

1 Introduction

The present approach to the problem of the definition of path integrals is a generalization of the standard stationary phase method: the contributions are given by the exact solutions of the equation

$$\delta\bar{S}=0, \tag{1. 1}$$

where the action $\bar{S}$ includes a random source of quantum perturbations.

In quantum theories one often encounters problems where the boundary conditions for Eq.(1. 1) are missing. We shall use an additional selection rule which amounts to the following: those quantum processes are important which correspond to the largest classical measure. The derivation of this rule is the main purpose of the present paper. To this end (see Ref. [1]) we shall find the connection with the classical description (Sec.2) and then (Ref.[2]), using a quantum-mechanical example, shall show the role played by the classical definition of measure in quantum processes.

The technical aspect of this idea is the suggestion to calculate directly the probability, which has a classical interpretation, avoi9ding the intermediate step of the calculations the amplitudes. in present paper we confine ourselves to the simplest problem - the motion of one particle in a potential $V(x)$. We shall use the semiclassical approximation since the result are independent of the magnitude of the quantum corrections. All our results can be derived by the methods of quantum mechanics, and the example discussed serves only as an illustration of our approach.

Let the amplitude $A(x_2,T;x_1,0)$ describe the motion of the particle from the point x_1 to the point x_2 during the time T. Using the spectral representation

$$A(x_2,T;x_1,0)=\sum_n \psi_n(x_2)\psi_n^*(x_1)e^{iE_nT}, \tag{1. 2}$$

for the probability we have:

$$W(x_2,T;x_1,0)=\sum_{n_1,n_2} \psi_n(x_2)\psi_n^*(x_1)\psi_n^*(x_2)\psi_n(x_1)e^{i(E_{n_1}-E_{n_2})T}. \tag{1. 3}$$

If one takes into account the condition of orthogonality

$$\int dx\psi_n(x)\psi_m^*(x)=\delta_{n,m}, \tag{1. 4}$$

then the quantity

$$\int dx_2 dx_1 W(x_2,T;x_1,0) = \sum_n = \int \frac{dxdp}{2\pi} = \Omega^2 \qquad (1.\ 5)$$

is the independent of T and coincides with the number of states, or, in the semiclassical approximation, with the volume of the phase space of one particle. In Sec.2 we show the connection between the classical and quantum descriptions and derive Eq.(1. 5).

In Sec.3 we consider the role of the conservation laws. Thus, the Fourier transform of $A(x_2,T;x_1,0)$ with respect to T

$$a(x_2,x_1;E) = \sum_n \frac{\psi_n(x_2)\psi_n^*(x_1)}{E-E_n-i0} \qquad (1.\ 6)$$

leads to probability

$$\omega(x_2,x_1;E) = \sum_{n_1,n_2} \frac{\psi_n(x_2)\psi_n^*(x_1)}{E-E_{n_1}-i0}\frac{\psi_n^*(x_2)\psi_n(x_1)}{E-E_{n_2}+i0}. \qquad (1.\ 7)$$

From this one has

$$\bar{\omega}(E) = \int dx_1 dx_2 \omega(x_2,x_1;E) = \sum_n \left| \frac{1}{E-E_n-i0} \right|^2 =$$

$$= \frac{1}{0}\sum_n \mathrm{Im}\frac{1}{E-E_n-i0} = \Omega \sum_n \delta(E-E_n), \qquad (1.\ 8)$$

where $\omega = 1/0 = \infty$. We shall show that this infinite coefficient is a consequence of the translational invariance of the problem with respect to time. As expected, the conservation laws reduce the number of the degrees of freedom, which is reflected in the different number of zero modes in (1. 8) and (1. 5).

The appearance of infinities in (1. 8) and (1. 5) shows that the contributions discussed are realized on the largest measure. This question is discussed more fully in Sec.4. Finally, the results of the paper are summarized up in Sec.5.

2 The generalized stationary-phase method

Calculating the quantity

$$|A|^2 = <\mathrm{in}|\mathrm{out}><\mathrm{in}|\mathrm{out}>^* = <\mathrm{in}|\mathrm{out}><\mathrm{out}|\mathrm{in}>, \qquad (2.\ 1)$$

one can show that the converging and diverging waves interfere in such a way that some of the contributions to $|A|^2$ cancel each other [1]. In order to see this it is convenient to write the amplitude in terms of path integrals:

$$A(x_2,T;x_1,0) = \int_{x(0)=x_1}^{x(T)=x_2} \frac{Dx}{C_T} e^{-iS_T(x)}, \qquad (2.\ 2)$$

where the action S_T is gien by

$$S_T(x) = \int_0^T dt \left(\frac{1}{2}\, \dot{x}^2 - V(x) \right) \tag{2. 3}$$

and C_T is the standard normalization coefficient:

$$C_T = \int_{x(0)=x_1}^{x(T)=x_2} \exp\{-\frac{i}{2} \int_0^T dt\ \dot{x}^2\} \tag{2. 4}$$

Let us calculate the quantity

$$W(x_2, T; x_1, 0) = \int_{x(0)=x_1}^{x(T)=x_2} \frac{Dx_+}{C_T} \frac{Dx_-}{C_T^*} e^{-iS_T(x_+)+iS_T(x_-)} \tag{2. 5}$$

For simplicity below we assume that in (2. 2) the integration is over trajectories for which the action is real.

In order to to take into account explicitly the interference between the contributions of the trajectories $x_+(t)$ and $x_-(t)$ we shall go over from the integration over two independent trajectories x_+ and x_- to the pairs (x, e):

$$x_|pm(t) = x(t) \pm e(t). \tag{2. 6}$$

Upon this substitution of (2. 6) into (2. 5), the argument of the exponent takes the form

$$S_T(x+e) - S_T(x-e) 2 \int_0^T dte(\ddot{x} + V'(x)) - \tilde{S}_T(x, e), \tag{2. 7}$$

where $\tilde{S}_T(x, e)$ is the remainder of the expansion in powers of $e(t)$ ($\tilde{S}_T = O(e^3)$). Note that in (2. 7) we have discarded the "surface" term

$$\int_0^T dt \partial_t (e\dot{x}) = e(T)\dot{x}(T) - e(0)\dot{x}(0) = 0, \tag{2. 8}$$

since the boundary points of the trajectories $x_+(0) = x_-(0) = x_1$ and $x_+(T) = x_-(T) = x_2$ are not varied:

$$e(o) = e(T) = 0. \tag{2. 9}$$

Next,

$$Dx_+ Dx_- = JDxDe, \tag{2. 10}$$

where J is an unimportant Jacobian of the transformation.

As a result of the replacement (2. 6) we have

$$W(x_2, T; x_1, 0) = \int_{x(0)=x_1}^{x(T)=x_2} \frac{Dx}{|C_T|^2} \int_{x(0)=0}^{x(T)=0} De\ \exp\left\{ 2i \int_0^T dte(\ddot{x} + V'(x)) + \tilde{S}_T(x, e) \right\}. \tag{2. 11}$$

One can make use of the formulae

$$e^{i\tilde{S}_T(x,e)} = \hat{e}(e', j) e^{i\tilde{S}_T(x,e')} \exp\{-2i \int_0^T e(t) j(t) dt\}, \tag{2. 12}$$

where we have introduced the operator

$$e(e',j) = \lim_{e=j=0} exp\{-\frac{1}{2i}\int_0^T \frac{\delta}{\delta j(t)}\frac{\delta}{\delta e(t)}\}, \qquad (2.\ 13)$$

after which from (2. 10) we have found that

$$W(x_2,T;x_1,0) = J\hat{e}(e',j)\int_{x(0)=x_1}^{x(T)=x_2} \frac{Dx}{|C_T|^2} e^{i\tilde{S}_T(x,e')}\times$$

$$\times \int_{x(0)=0}^{x(T)=0} De\ \exp\left\{2i\int_0^T dt(\ddot{x}+V'(x)-j)e\right\} =$$

$$= J'\hat{e}(e,j)\int_{x(0)=x_1}^{x(T)=x_2} \frac{Dx}{|C_T|^2} e^{i\tilde{S}_T(x,e)}\prod_{t\neq 0,T}\delta(\ddot{x}+V'(x)-j), \qquad (2.\ 14)$$

where the functional δ-function

$$\prod_{t\neq 0,T}\delta(\ddot{x}+V'(x)-j) = \frac{J}{J'}\int_{x(0)=0}^{x(T)=0} De\ \exp\left\{2i\int_0^T dt(\ddot{x}+V'(x)-j)e\right\} \qquad (2.\ 15)$$

has arisen as a result of total reduction of the contributions of the trajectories that are unphysical for the classical equation of motion

$$\ddot{x}(t)+V'(x) = j(t). \qquad (2.\ 16)$$

Note that this equation can be obtained by variation of the effective action

$$\bar{S}(x) = S_T(x) + \int_0^T dt x(t)j(t),$$

where $j(t)$ is an external perturbation force. Following the definition of the operator (r2.13), we must turn out attention to the expansion of the solutions of the Eq.(2. 16) in powers of $j(t)$. Let us note also that the operator (2. 13) is Gaussian, so that we can assume that the system under consideration is perturbed by a random force $j(t)$ (in this connection see [2]).

The qualitative side of the derivation of the exact formulae (2. 14) is as follows. By virtue of the derivation of the definition of W, the difference $S_T(x_+) - S_T(x_-)$ in (2. 5) coincides with the action during the cycle, so that by definition we are only interested in reversible processes. Upon the substitution (2. 6) we have identified the "true" trajectory $x(t)$ and the virtual deviation $e(t)$. Then the quantity $e(\ddot{x}+V'(x)-j)$ coincides with virtual work. By contrast to classical mechanics one has to integrate over $e(t)$, as a result of which the measure of the remaining path integral takes a Dirac δ-function form. In other words, the proposed definition of the measure of the path integral is similar to the classical d'Alembert's principle. As is known, on the basis of this principle the theory can take into account any external perturbations [in our case, the perturbation introduced by the source $j(t)$].

In the semiclassical approximation $\hat{e}(e,j)$ is given by the $j\to 0$ limit, and thus from (2. 14) we find that

$$W(x_2,T;x_1,0) = J'\hat{e}(e,j)\int_{x(0)=x_1}^{x(T)=x_2} \frac{Dx}{|C_T|^2}\prod_{t\neq 0,T}\delta(\ddot{x}+V'(x)), \qquad (2.\ 17)$$

Let the solution of the homogeneous equation

$$\ddot{x} + V'(x) = 0 \tag{2. 18}$$

be $x_c(t)$, with $x(0) = x_1$ and $x(T) = x_2$. Then

$$W(x_2, T; x_1, 0) = J'\hat{e}(e, j) \int_{x(0)=x_1}^{x(T)=x_2} \frac{Dx}{|C_T|^2} \prod_{t \neq 0,T} \delta(\ddot{x} + V''(x_c)x), \tag{2. 19}$$

The remaining integral is calculated by the standard methods [3] (here it is more convenient to represent (2. 19) as a production of two Gaussian integrals). As a result we find

$$W(x_2, T; x_1, 0) = \frac{1}{2\pi} \left| \frac{\partial^2 S_T(x_c)}{\partial x_c(0) \partial x_c(T)} \right|_{x_c(0)=x_1, x_c(T)=x_2}. \tag{2. 20}$$

Next, let us recall that the full derivative of the classical action is

$$dS = p_2 dx_2 - p_1 dx_1, \tag{2. 21}$$

where p_2 and p_1 are, respectively, the final and initial momentum. Then, however,

$$\left| \frac{\partial^2 S_T}{\partial x_1 \partial x_2} \right| dx_2 = dp_1, \tag{2. 22}$$

as a result of which we see that

$$\int dx_1 dx_2 W(x_2, T; x_1, 0) = \int \frac{dx_1 dx_2}{2\pi} = \Omega^2, \tag{2. 23}$$

which coincides with (1. 5).

In the derivation of (2. 23) we have simplified the problem somewhat by considering a unique solution of Eq.(2. 16). A more complete solution of the problem is given in the next section. Here it was only important to demonstrate that the contributions to the functional integrals are determined by the exact solution of the classical equation (2. 16), which we interpret as a connection between the classical and quantum descriptions independently of the magnitude of the quantum corrections.

3 Taking the conservation laws into account

Let us consider the motion in the phase space. To this end, we substitute into (2. 2) the equalities

$$1 = \int \frac{Dp}{B_T} \exp\left\{ -\frac{i}{2} \int_0^T dt (p - \dot{z})^2 \right\}, \quad B_T = \int Dp \exp\left\{ -\frac{i}{2} \int_0^T dt p^2 \right\}. \tag{3. 1}$$

Then

$$a(x_1, x_2; E) = \int_0^\infty dT e^{-ieT} A(x_2, T; x_1, 0) =$$

$$= \int_0^\infty dT e^{-ieT} \int_{x(0)=x_1}^{x(T)=x_2} \frac{Dx Dp}{Z_T^2} \exp\{-iS_T(x, p)\}, \tag{3. 2}$$

where the action S_T is given by

$$S_T(x,p) = \int_0^T dt(p\dot{x} - H(p,x)) \qquad (3.\ 3)$$

and H is the Hamiltonian

$$H(p,x) = 1/2p^2 + V(x). \qquad (3.\ 4)$$

The normalization coefficient is

$$Z_T = \int DxDp \exp\left\{-\frac{i}{2}\int_0^T (p_2 - 2p\dot{x})\right\}. \qquad (3.\ 5)$$

Below we shall study the simplest example, where the potential has a single minimum at $x = 0$.

Proceeding in the some way as in the derivation of (2. 14), we calculate $|a(x_1, x_2; E|^2$ and then integrate over x_1 and x_2. As a result, in the semiclassical approximation we obtain

$$\bar{\omega}(E) = \lim_{j=0} \int_0^\infty \frac{DxDp}{|Z_T|^2} e^{-iS_0(p,x)} \delta(E - H(p,x)) \times$$
$$\times \prod_t \delta\left(\dot{p} + \frac{\partial H}{\partial x} - j\right) \delta\left(\dot{x} - \frac{\partial H}{\partial p}\right), \qquad (3.\ 6)$$

where

$$S_0(p,x) = \lim_{t=0}(S_{T+t}(p,x) - S_{T-t}(p,x)) \qquad (3.\ 7)$$

can be different from zero if the trajectory is a periodic one (note that in the preceding section the time T was fixed and therefore $S_0 = 0$ independently of the type of the trajectory). In (3. 6) we have also taken into account that $\partial_T S_T = -H$.

In order to calculate the remaining integrals in (3. 6) we must find all solutions of the equations

$$\dot{p} + \frac{\partial H}{\partial x} = j, \quad \dot{x} - \frac{\partial H}{\partial p} = 0 \qquad (3.\ 8)$$

in the vicinity of the point $j = 0$. First, for the potential chosen these equations have the "trivial" solution

$$x_1(t|j = 0) = 0, \quad p_1(t|j = 0) = 0, \qquad (3.\ 9)$$

which in the semiclassical approximation corresponds to a particle at rest at the bottom of the potential well. Expanding $x_1(t|j)$ and $p_1(t|j)$ in powers of $j(t)$ [under the condition (3. 9)], we obtain an expansion in powers of the nonlinearity of the potential $V(x)$. It is not difficult to see that this expansion corresponds to the standard perturbation theory (the proof of this statement in the field theory will be given in our next paper) and describes the Brownian motion of the particle under the influence of the perturbing force $j(t)$. Below this contribution to $\bar{\omega}(E)$ will be denoted by $\bar{\omega}_1(E)$.

Another solution of the equation (3. 8) is a purely periodic trajectory $(x_2, p_2) = (x_c, p_c) + O(j)$, where the orbit (x_c, p_c) [not perturbed by the source $j(t)$] is an exact nontrivial solution of the equations

$$\dot{p} + \frac{\partial H}{\partial x} = 0, \quad \dot{x} - \frac{\partial H}{\partial p} = 0 \qquad (3.\ 10)$$

of classical mechanics. This equations are translationally invariant. Therefore

$$x_c = x_c(t+t_0,\epsilon), \quad p_c = p_c(t+t_0,\epsilon), \tag{3. 11}$$

where ϵ is the energy of the particle on the trajectory (x_c, p_c):

$$H(x_c, p_c) = \epsilon. \tag{3. 12}$$

The integration in (3. 6) is performed over all the trajectories, which implies integration over ϵ and t_0 as well (recall that T is the proper time). In other words,

$$\bar{\omega}_2(E) = \int dt_0 \delta\epsilon \delta(E-\epsilon) \int_0^\infty dT \exp\{-iS_0(p_c,x_c)\}\times$$
$$\times \int \frac{DxDp}{|Z_T|^2} \prod_t \delta\left(\dot{p} + \frac{\partial H}{\partial x}\right) \delta\left(\dot{x} - \frac{\partial H}{\partial p}\right). \tag{3. 13}$$

Here

$$|Z_T|^2 = \int DxDp \prod_t \delta(\dot{x}-p)\delta(\dot{p}). \tag{3. 14}$$

Since we are considering a "two-particle" problem with a potential independent of time, we can always make a canonical transformation $(x,p) \to (X,P)$

$$DxDp = DXDP, \tag{3. 15}$$

such that

$$\dot{P} = -\frac{\partial H'}{\partial X} = 0, \quad \dot{X} = \frac{\partial H'}{\partial P} = const, \tag{3. 16}$$

where H' is the transformed Hamiltonian. The new variables have the meaning of the action-angle variables. Upon such a transformation, taking into account the fact that (x_c, p_c) ia a periodic trajectory, we obtain

$$\bar{\omega}_2(E) = \int dt_0 \delta\epsilon \delta(E-\epsilon) \int_0^\infty dT \Phi_T \exp\{-iS_0(p_c,x_c)\}, \tag{3. 17}$$

where Φ_T is a phase factor which takes into account the periodicity of the contribution [4].

Next, because H has a constant sign, for periodic trajectory one has

$$S_)(p_c,x_c) = \int_T^T dt p_c \dot{x}_c = \oint_{x_c} pdx \tag{3. 18}$$

[which takes into account the uncertainty in taking the limit $t \to 0$ in (3. 7)]. In the formula (3. 18)

$$p = \pm[2(\epsilon - V(x))]^{1/2}. \tag{3. 19}$$

Since x_c is a periodic function, one can write

$$\int_0^\infty dT f_T(x_c) = \sum_{n=0}^\infty \int_0^{T_1} dT f_{T+nT_1} \tag{3. 20}$$

where T_1 is the period:

$$T_1(\epsilon) = 2\int_{z_-}^{z_+} \frac{dz}{[2(\epsilon - V(z)]^{1/2}}, \quad V(z_\pm) = \epsilon. \tag{3. 21}$$

Taking into account (3. 20) and the fact that $\oint pdx$ is independent of the integration path, we have

$$\oint_{z_c(T+nT_1)} pdx = \pm 2n \int_{z_-}^{z_+} dz[2(\epsilon - V(z)]^{1/2} \equiv \pm n S_1(\epsilon). \tag{3. 22}$$

As a result, from (3. 17) we find that

$$\bar{\omega}_2(E) = \Omega T_1(E) \sum_{n=0}^{\infty} (-1)^n \left(e^{-iS_i(E)n} + e^{iS_i(E)n}\right), \tag{3. 23}$$

where

$$\Omega = \int dt_0 \tag{3. 24}$$

is the volume of the translational group of the Hamiltonian H. The formulae (3. 23) also takes into account that $\Phi_{nT_1} = (-1)^n$.

In (3. 23) we have to complete the definition of the sum over n by the standard prescription $E \to E - i0$. Then

$$\bar{\omega}_2(E) = \Omega T_1(E) \left\{ \frac{1}{1 + e^{-iS_1 - 0}} + \frac{1}{1 + e^{iS_1 - 0}} \right\} = \Omega \sum_n \delta(E - E_n), \tag{3. 25}$$

since [see the formulae (3. 21)] $\partial S_1(E)/\partial E = T_1(E)$; E_n is defined by the usual Bohr-Sommerfeld quantization rule

$$S_1(E_n) = 2\int_{z_-}^{z_+} dz[2(E_n - V(z))]^{1/2} \equiv \pi(2n+1). \tag{3. 26}$$

Summing the formulae obtained, from (3. 6) we obtain

$$\bar{\omega}(E) = \bar{\omega}_1(e) + \Omega \sum_{n=0}^{\infty} \delta(E - E_n) = \Omega \sum_{n=0}^{\infty} \delta(E - E_n)(1 + O(1/\Omega)), \tag{3. 27}$$

which demonstrate the dominance of the contribution of the periodic trajectories. In other words, we have shown that the standard periodic boundary conditions for the Schrodinger equation for a particle in a potential well select the only probable forms of motion.

4 Selection rules

Let us generalize the above result to systems with a large number of degrees of freedom. If the trajectory fills densely the $2N$-dimensional phase space volume, then by virtue of

the invariance of the equations of motion and of the measure $D^N x D^N p$ under canonical transformations, the quantity

$$\int d^N x_1 d^N x_2 W(x_2, T; x_1, 0) = \Omega^{2N} \quad (4.\ 1)$$

coincides with the number of states in the phase space. This follows from the fact that one can always perform a canonical transformation [being in the frame of semiclassical approximation] as a result of which the dependence on the initial conditions disappears. Here it is important that the integration is performed over all trajectories, which differ also in their initial condition (see Sec.2). This demonstrates the dominance of the ergodic fluxes in the phase space for quantum mechanical problems.

Let us discuss the role of the conservation laws. If the system is integrable, i.e. if there exist N first integrals of motion, then in the @N-dimensional phase space the system occupies a smaller volume: when one makes the canonical transformation to the action-angle variables, the trajectory wraps around the surface of an N-dimensional hypertorus. Then, repeating the arguments above, we find that the corresponding probability is

$$\sim \Omega^N \quad (4.\ 2)$$

The system with $2N = 2$ degrees of freedom studied in Sec.3 is fully integrable (in the semiclassical approximation), there is one integral of motion (the energy), and therefore the probability is $\sim \Omega^1$. In quantum mechanics the dominant motion is the motion in the resonant tori, as the result of which the energy is quantized. Finally, if the Hamilton equations have only the trivial solutions $x(t|j = 0) = 0$, $p(t|j = 0) = 0$, i.e. if the motion is made possible only as a result of quantum perturbations, then the probability is

$$\sim \Omega^0, \quad (4.\ 3)$$

since in the semiclassical approximation the volume that the trajectory occupies in the phase space is zero.

Therefore, taking into account the definition of the quantum-mechanical probability one can establish a one-valued correspondence between the classical and quantum and, thus, introduce the classical definition of measure into quantum theory. Here we note an advantage of the approach based on functional integration.

Then in our approach the problem of quantization of an arbitrary Lagrange theory is divided into two parts:

(a) one must know exactly all the regular solutions of the equation of motion (the solutions must be regular since the definition of probability implies the reversibility of motion ant therefore in the variation of action the surface terms must be discarded; the solution have to be exact since there is complete cancellation of the contributions of the trajectories that are unphysical for the non-homogeneous equation of motion);

(b) from the sum of the contributions of all such solutions one must select those that lead to the motion (in the classical sense) in the largest volume of the phase space, i.e. which are realized on the largest measure.

5 Conclusion

Let us state the main results of the paper.

1. All the calculations must be performed in the space with the Minkowski metric. This condition is important in the field theories with a high group symmetries (such as the theories of the Yang-Mills type) since for such theories one has yet not been able to perform adequately the analytic continuation into the Euclidean region. (The fact that a theory must satisfy certain conditions upon analytic continuation in time is clear from [5].) Apart from that, in the pseudo-Euclidean metric one is able to take into account external conditions with nontrivial time dependence without any restrictions.

2. The quantization can be performed without the transition to the canonical formalism (see Sec.2), remaining in the Lagrange formalism which is a more natural formalism for relativistic field theories.

3. In obtaining the contributions to the functional integrals onle the exact solutions of the equation of motion must be taken into account.

4. The contributions to functional integrals are found by variation of the classical nonrenormalized action, which simplifies the calculations considerably. This important feature of our approach is discussed in forthcoming publications in the light of the phenomenon of spontaneous symmetry breaking.

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